HL 20.5-6 – Reaction Pathways and Stereoisomerism

IB Chemistry
T10D13
Mr. Martin Brakke

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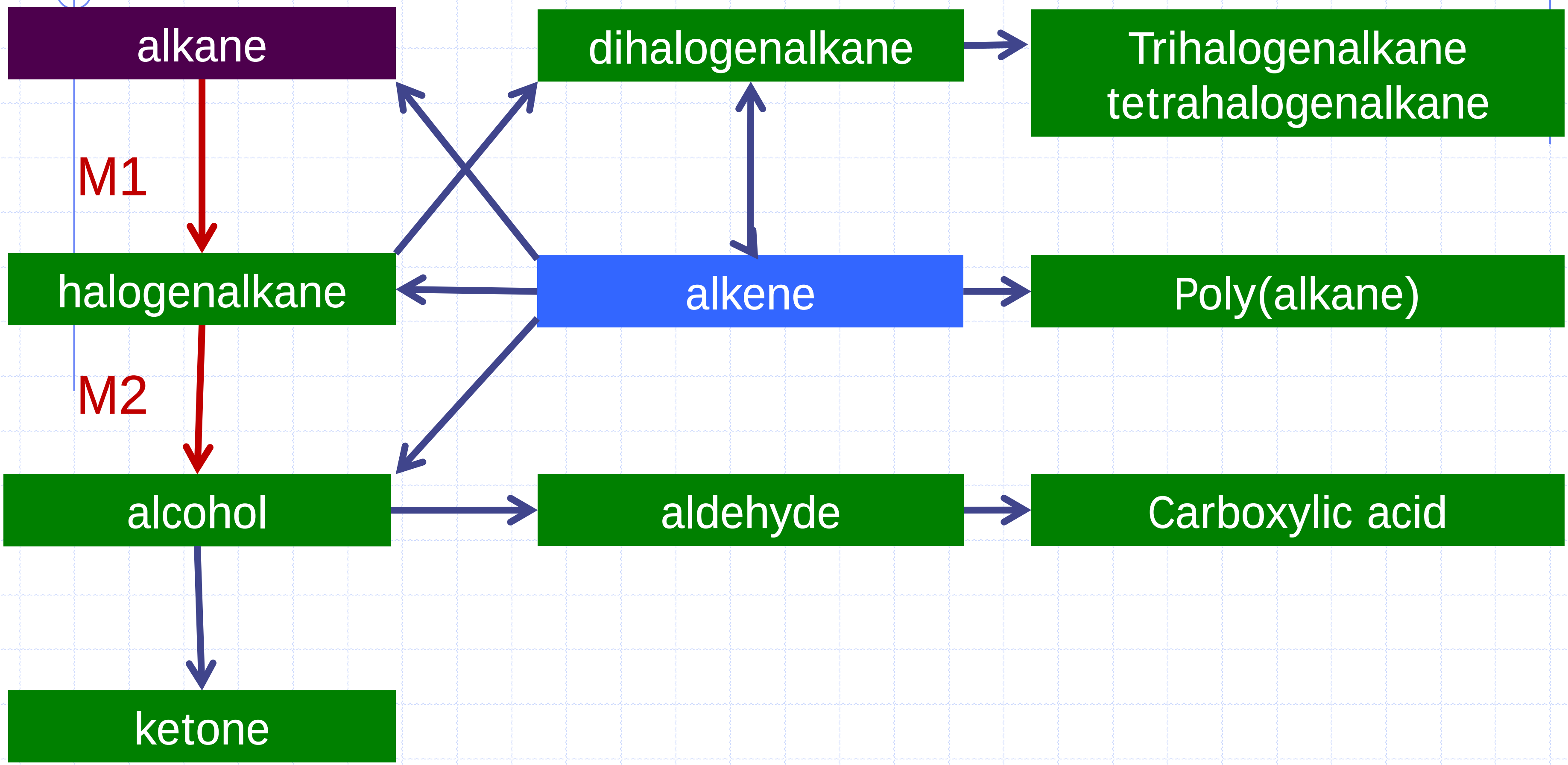
Reaction Pathways

10.6.1 Deduce reaction pathways given the starting materials and the product. (3)



For the IB Exam you need to know the following **mechanisms**

M1 – Halogen / UV light

M2 – NaOH

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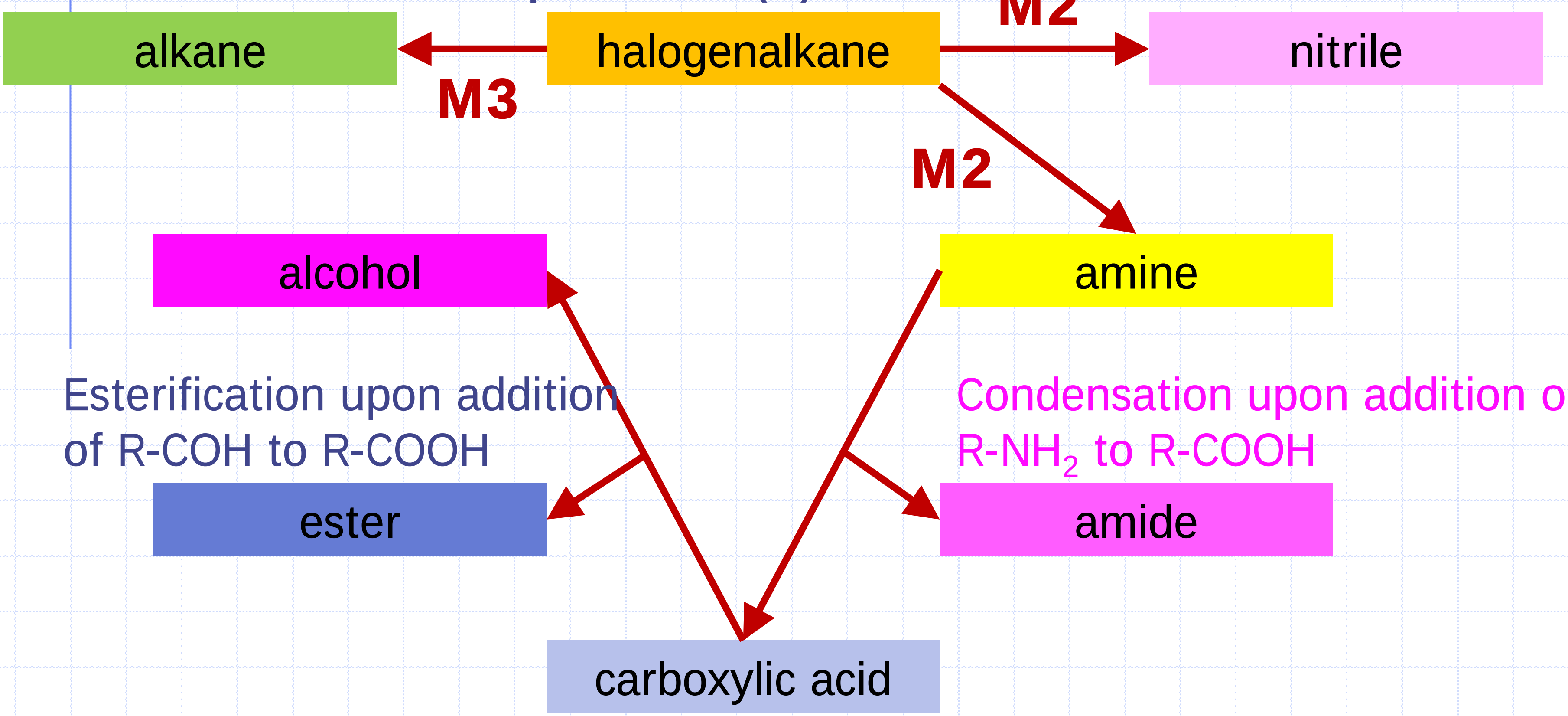
20.5 – Reaction Pathways

- 20.5.1 Deduce reaction pathways given the starting materials and the product. (3)



M1: Topic 10.2 – Free Radical substitution with Cl_2 (halogen) and UV light
M2: S_N1 or S_N2 mechanism with CN^- or NH_3 nuclophiles
M3: E1 or E2 elimination of Halogen, then hydrogenation of the double bond

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20.6 – Stereoisomerism

- 20.6.1 Describe stereoisomers as compounds with the same structural formula but with different arrangements of atoms in space. (2)
- 20.6.2 Describe and explain geometrical isomerism in non-cyclic alkenes. (3)
- 20.6.3 Describe and explain geometrical isomerism in C3 and C4 cycloalkanes. (3)
- 20.6.4 Explain the difference in the physical and chemical properties of geometrical isomers. (3)
- 20.6.5 Describe and explain optical isomerism in simple organic molecules. (3)
- 20.6.6 Outline the use of a polarimeter in distinguishing between optical isomers. (2)
- 20.6.7 Compare the physical and chemical properties of enantiomers. (3)

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Stereoisomers

20.6.1 Describe stereoisomers as compounds with the same structural formula but with different arrangements of atoms in space. (2)

- **Structural isomers** are compounds with the same molecular formula but different structural formulas
  - Propan-1-ol vs propan-2-ol (C_3H_8OH)
  - Butane vs 2-methylpropane (C_4H_{10})
- If molecules have the same molecular formula AND the same structural formula but there atoms are arranged in different directions in space, they are known as **stereoisomers**.
  - Geometrical Isomerism (20.6.2-4)
  - Optical Isomerism (20.6.5-6)

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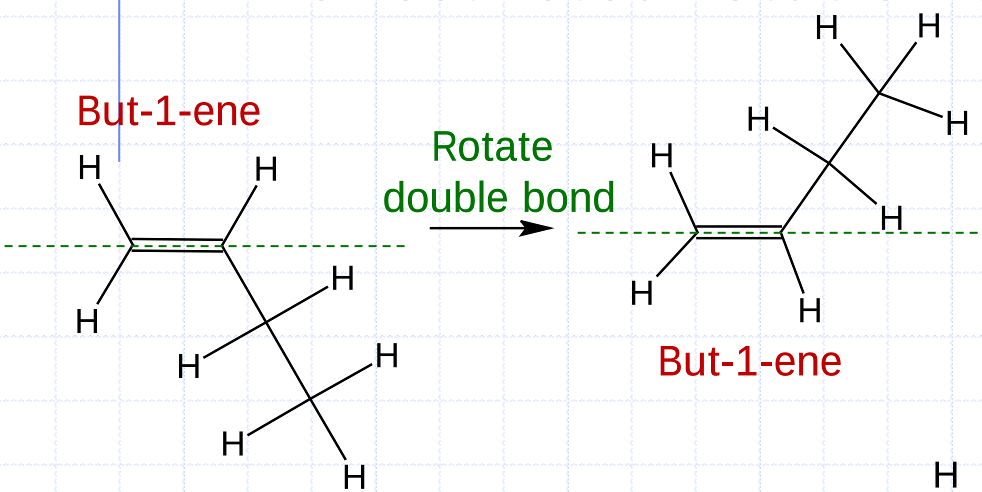
Geometrical Isomers of Non-Cyclics

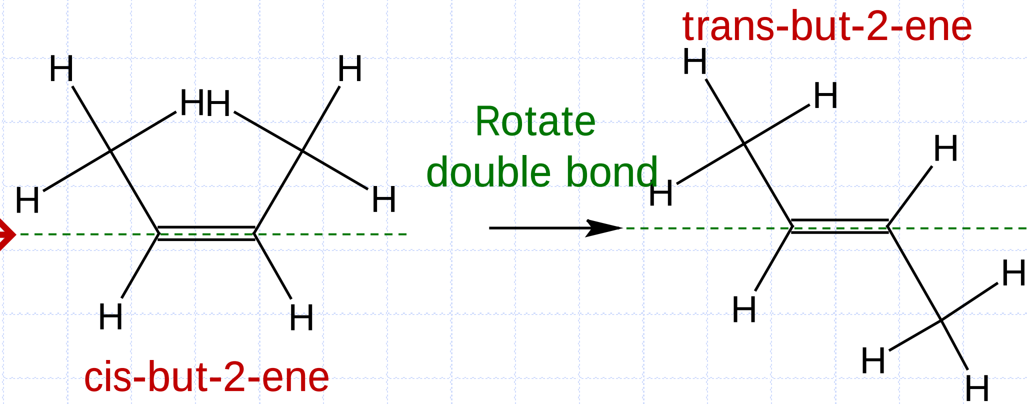
20.6.2 Describe and explain geometrical isomerism in non-cyclic alkenes.

- **Geometrial Isomerism** occurs when the arrangement of the bonds prevents free rotation around the axis through the molecule
  - The **restricted rotation** occurs in alkenes for example:



←NOT Geometrical isomers

Geometrical isomers →



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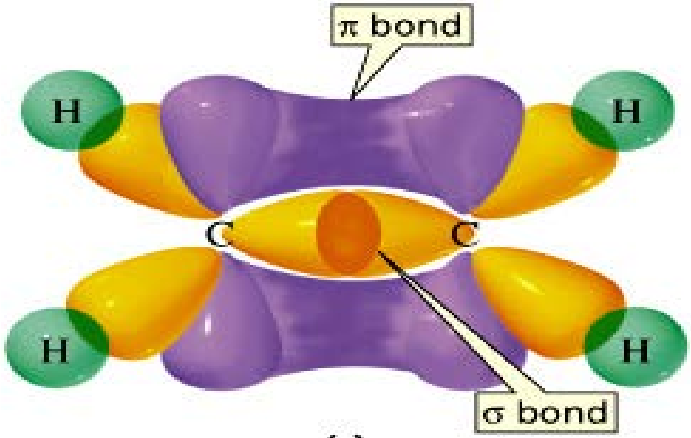
Rotation of Single vs Double

- In a single bond (sp^3) , there is free rotation the head-to-head overlap of sigma (σ) bonds does not provide any hindrance so long each side chain (R group) is equal.

- When a double bond (sp^2) is present, the side-to-side overlap of the pi (π) bonds for the p-orbitals must remain in the same plane. To break this bond, considerable energy must be added. Therefore cis and trans are stable isomers.



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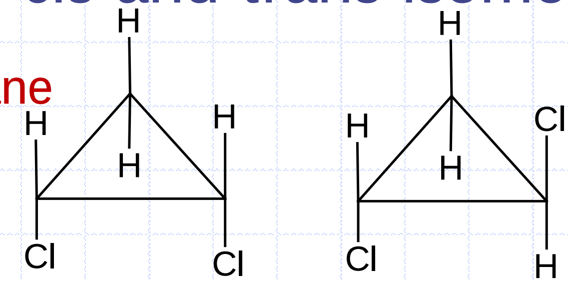
Geometrical Isomers of Cycloalkanes

20.6.3 Describe and explain geometrical isomerism in C3 and C4 cycloalkanes. (3)

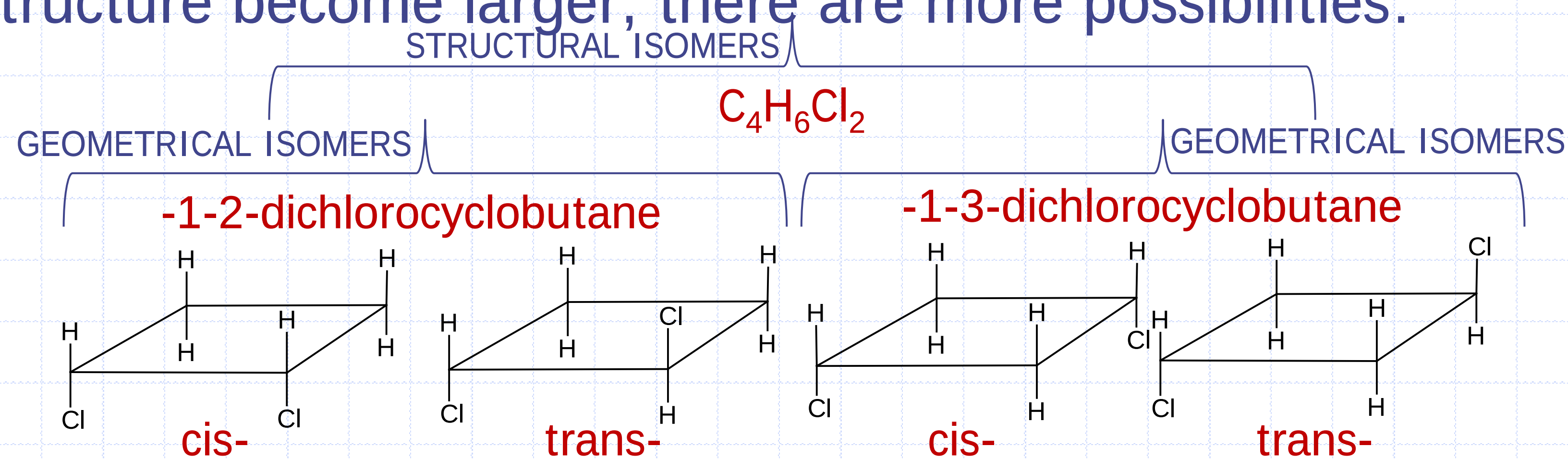
- Cyclic alkanes also restrict the free rotation of single bonds.
- Even though only single bonds are present between the c-atoms, the rigid structure prevents free rotation and we once again have cis and trans isomers

cis-1,2-dichlorocyclopropane



trans-1,2-dichlorocyclopropane

- As structure become larger, there are more possibilities:



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Properties of Isomers

20.6.4 Explain the difference in the physical and chemical properties of geometrical isomers. (3)

- In general, for geometrical isomers
  - The **trans** isomer has the higher melting point
  - The **cis** isomer has the higher boiling point

Isomer	Condensed Structure	Melting Point / K	Boiling Point / K
cis-but-2-ene	$CH_3CH=CHCH_3$	134	277
trans-but-2-ene	$CH_3CH=CHCH_3$	167	274
cis-1,2-dichloroethene	ClCH=CHCl	193	333
trans-1,2-dichloroethene	ClCH=CHCl	223	321

  - There must be stronger intermolecular forces present between cis isomers compared to trans
    - Van der Waals should be identical as they have the same composition
    - But where (direction) the substituents are affects polarity greatly

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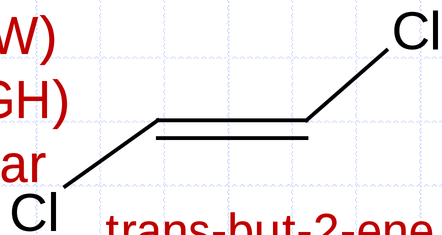
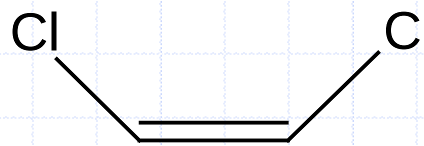
M.P. / B.P. of Isomers

- Let's take a look at the structures to explain this:

B.P. (LOW)
M.P. (HIGH)
Non-Polar



trans-but-2-ene



cis-but-2-ene

B.P. (HIGH)
M.P. (LOW)
Polar

- Why does –trans have a higher M.P.?
  - In order to be a solid compound the compound must pack together in a lattice structure, and –trans is much better due to its shape, where –cis is not as effective
- Why does –cis have a higher B.P.?
  - The polarity of the –cis isomer allows it to have dipole/dipole interactions (strong intermolecular forces)

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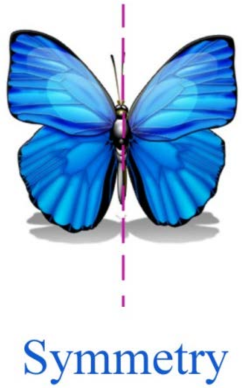
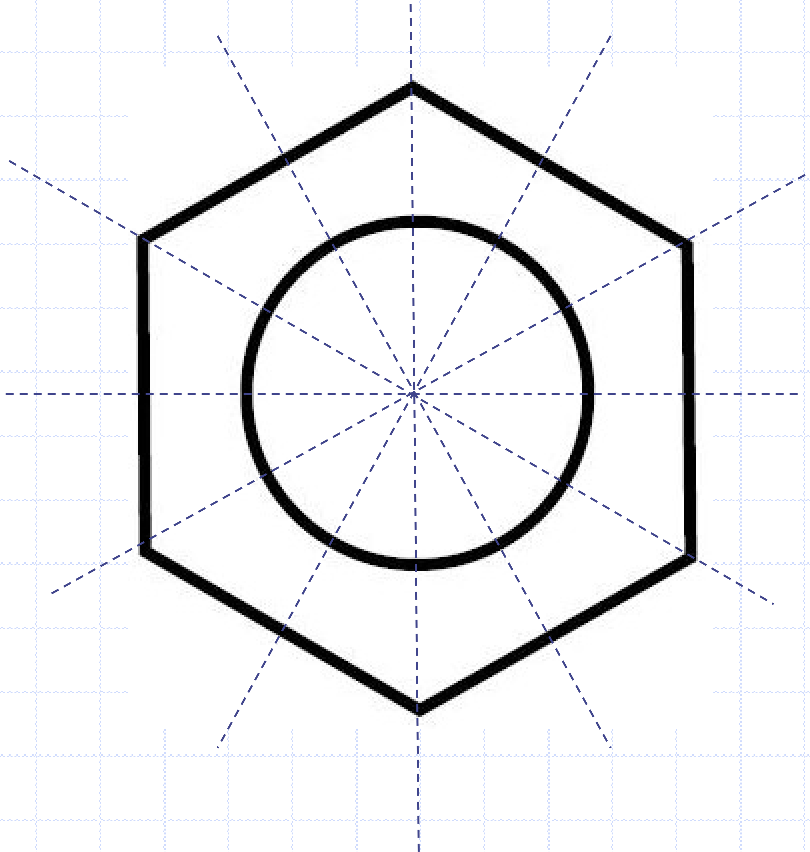
Optical Isomerism

20.6.5 Describe and explain optical isomerism in simple organic molecules.

- **Symmetry** is very apparent in come objects and not so much in others.
- The plane of symmetry can be demonstrated below:





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Chirality and Enantiomers

- **Optical Isomerism** arises from the inherent asymmetry of the molecules that make up each isomer.
  - The molecule can exist in left- and right-handed forms that are non-superimposable mirror images of each other: must posses a chiral center
- Molecules with no plane or center of symmetry are known as **chiral** molecules. The most common would be a tetrahedral molecule with four different terminal atoms
  - The central carbon atom is asymmetric

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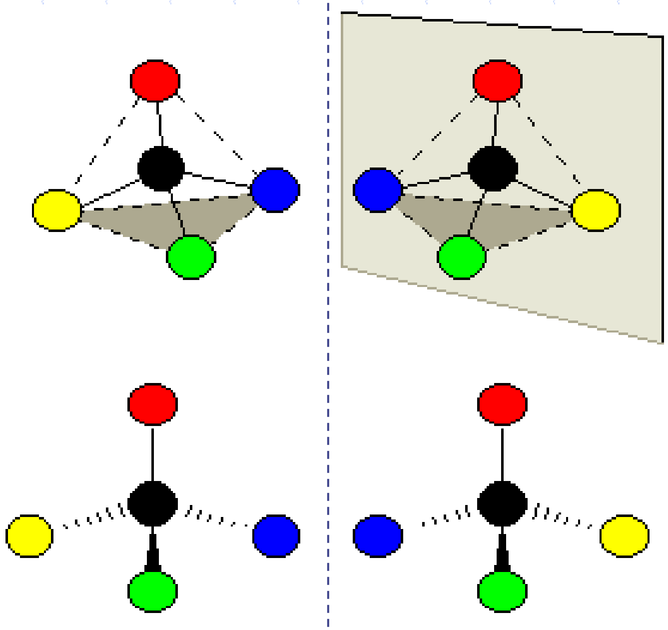
Enantiomers / Optical Isomers

- Molecules that mirror images of one another are known as **enantiomers** or **optical isomers**
- A **racemic mixture** is an equimolar mixture of two enantiomers of the same compound; as their rotation of plane-polarized light is equal but opposite, the mixture is not optically active.



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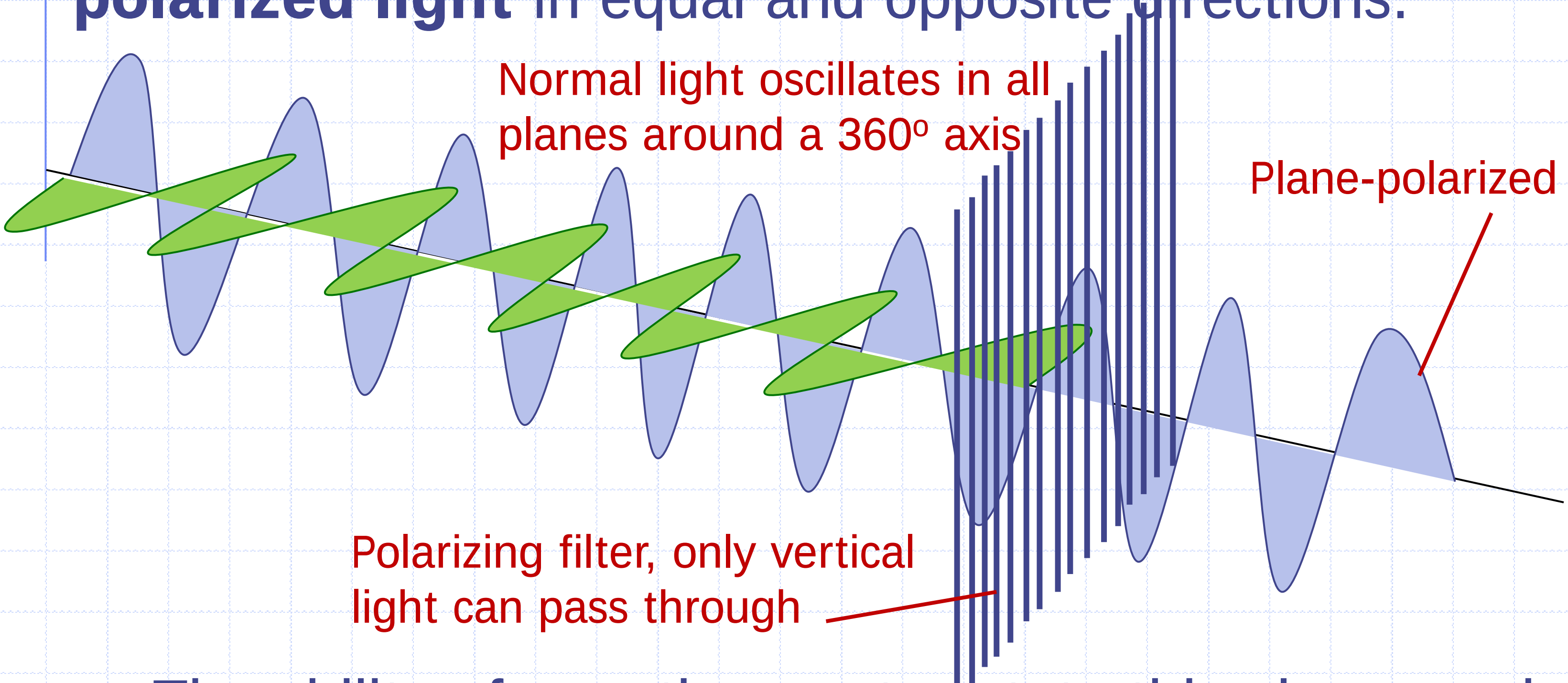
Polarimeter

20.6.6 Outline the use of a polarimeter in distinguishing between optical isomers. (2)

- The defining method used to distinguish between optical isomers of a compound is to rotate the plane of **plane-polarized light** in equal and opposite directions.



- The ability of enantiomers to rotate this plane can be shown using a **polarimeter**

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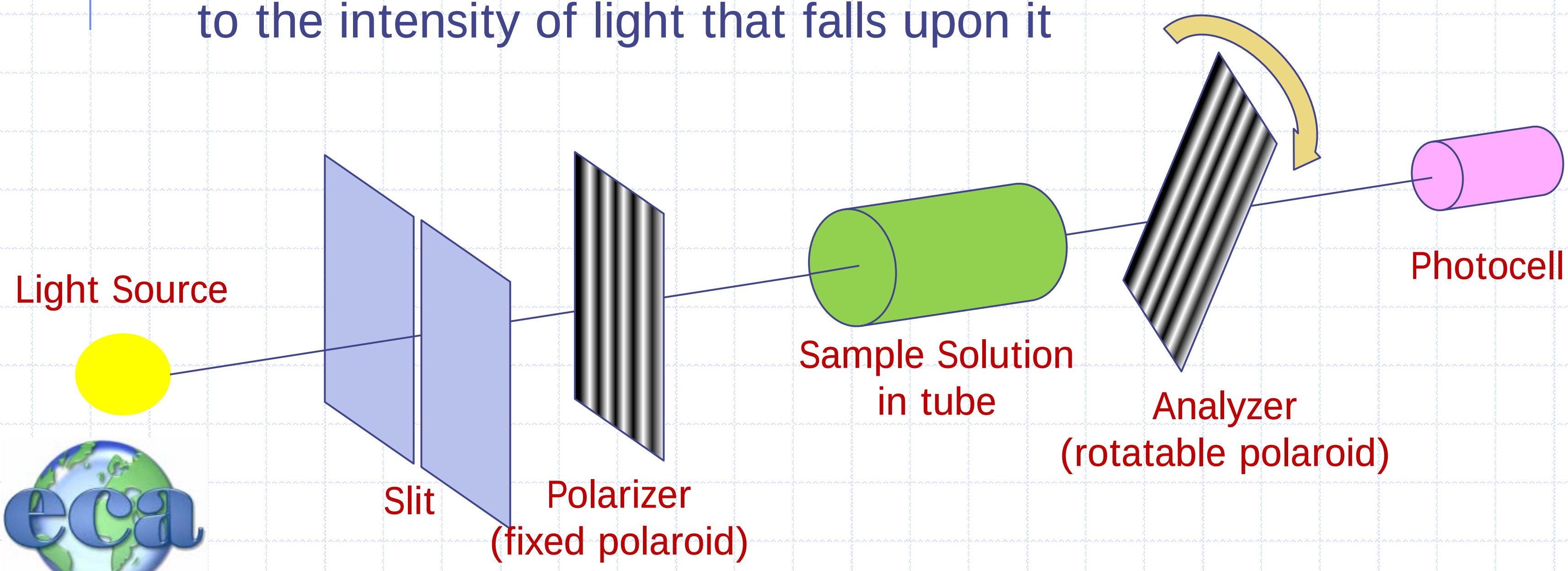
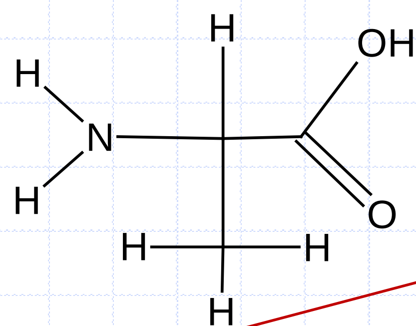
Polarimeter

- The **polarimeter** is used to distinguish optical isomers
  - Single wavelength light (monochromatic) passes through a slit to produce a thin beam of light
  - The beam passes through the Polaroid filter
  - Beam passed through sample
  - Beam through another Polaroid (the analyzer)
  - Beam enters the photocell producing an electric current proportional to the intensity of light that falls upon it



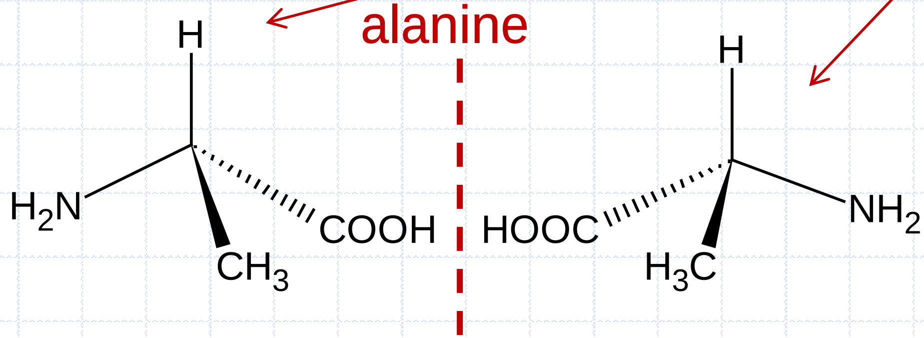
Optical Isomerism of 2-amino acids

- The 2-amino acids (in your data booklet) are used to synthesize proteins (long polymers)
- Of the 20 amino acids (10 essential / 10 non-essential) all but glycine are chiral molecules
  - Meaning they all have enantiomers



Each enantiomer rotates the plane-polarized light in opposite directions

alanine



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Properties of Enantiomers

20.6.7 Compare the physical and chemical properties of enantiomers. (3)

- The optical isomers differ in one defining physical property:
  - They rotate the plane of plan-polarized light in the opposite direction
- All other physical properties are identical
- All other chemical properties are identical
  - The only exception is when they interact with biological sensors
    - Amino acid Asparagine
      - One enantiomer tastes bitter
      - One enantiomer tastes sweet